



Full wwPDB EM Validation Report ⓘ

Nov 30, 2025 – 12:08 AM JST

PDB ID : 9KDH / pdb_00009kdh
EMDB ID : EMD-62276
Title : Cryo-EM structure of LIPID-mediated dimer of human norepinephrine transporter NET in the presence of Vanoxerine in an inward-open state at resolution of 2.52 angstrom
Authors : Zhang, H.; Xu, E.H.; Jiang, Y.
Deposited on : 2024-11-03
Resolution : 2.52 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

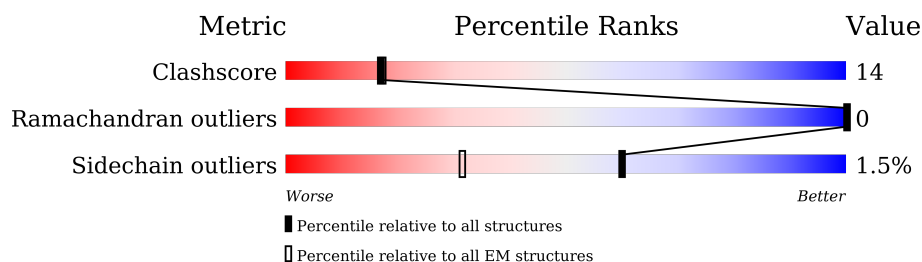
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.52 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	629	
1	B	629	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9470 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Sodium-dependent noradrenaline transporter.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	562	Total	C	N	O	S	0	0
			4470	2992	700	758	20		
1	B	562	Total	C	N	O	S	0	0
			4470	2992	700	758	20		

There are 24 discrepancies between the modelled and reference sequences:

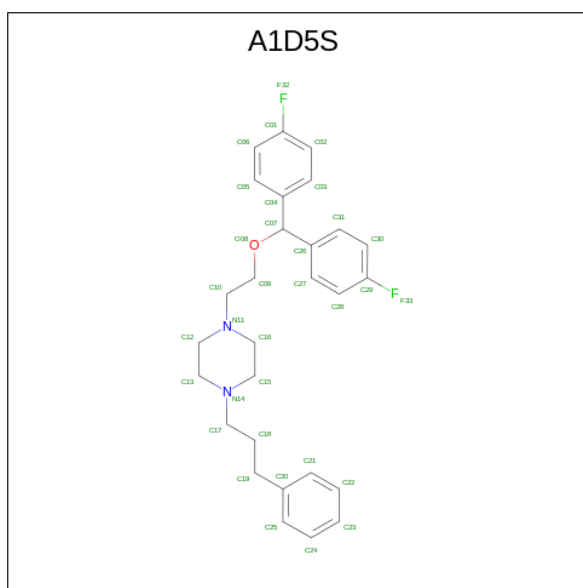
Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP P23975
A	-10	ASP	-	expression tag	UNP P23975
A	-9	TYR	-	expression tag	UNP P23975
A	-8	LYS	-	expression tag	UNP P23975
A	-7	ASP	-	expression tag	UNP P23975
A	-6	ASP	-	expression tag	UNP P23975
A	-5	ASP	-	expression tag	UNP P23975
A	-4	ASP	-	expression tag	UNP P23975
A	-3	LYS	-	expression tag	UNP P23975
A	-2	GLY	-	expression tag	UNP P23975
A	-1	SER	-	expression tag	UNP P23975
A	0	GLY	-	expression tag	UNP P23975
B	-11	MET	-	initiating methionine	UNP P23975
B	-10	ASP	-	expression tag	UNP P23975
B	-9	TYR	-	expression tag	UNP P23975
B	-8	LYS	-	expression tag	UNP P23975
B	-7	ASP	-	expression tag	UNP P23975
B	-6	ASP	-	expression tag	UNP P23975
B	-5	ASP	-	expression tag	UNP P23975
B	-4	ASP	-	expression tag	UNP P23975
B	-3	LYS	-	expression tag	UNP P23975
B	-2	GLY	-	expression tag	UNP P23975
B	-1	SER	-	expression tag	UNP P23975
B	0	GLY	-	expression tag	UNP P23975

- Molecule 2 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O).



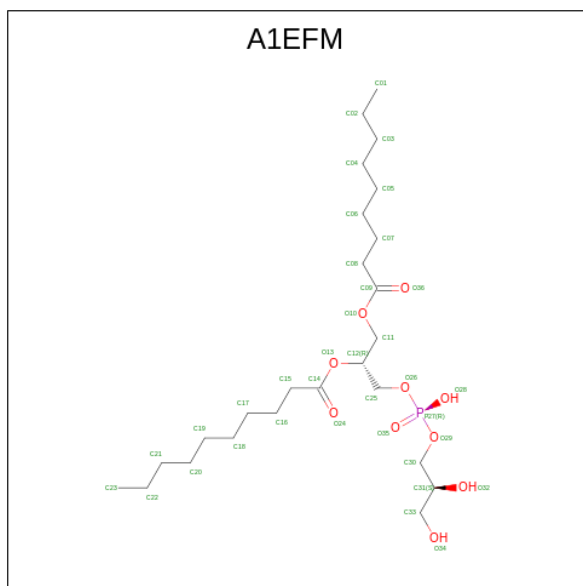
Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	C	O	0
			28	27	1	
2	A	1	Total	C	O	0
			28	27	1	
2	A	1	Total	C	O	0
			28	27	1	
2	A	1	Total	C	O	0
			28	27	1	
2	A	1	Total	C	O	0
			28	27	1	
2	A	1	Total	C	O	0
			28	27	1	
2	A	1	Total	C	O	0
			28	27	1	
2	B	1	Total	C	O	0
			28	27	1	
2	B	1	Total	C	O	0
			28	27	1	
2	B	1	Total	C	O	0
			28	27	1	
2	B	1	Total	C	O	0
			28	27	1	
2	B	1	Total	C	O	0
			28	27	1	
2	B	1	Total	C	O	0
			28	27	1	

- Molecule 3 is Vanoxerine (CCD ID: A1D5S) (formula: $C_{28}H_{32}F_2N_2O$).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	F	N	O	0
			33	28	2	2	1	
3	B	1	Total	C	F	N	O	0
			33	28	2	2	1	

- Molecule 4 is [(2 {R})-1-[(2 {S})-2,3-bis(oxidanyl)propoxy]-oxidanyl-phosphoryl]oxy-3-nonanoyloxy-propan-2-yl] decanoate (CCD ID: A1EFM) (formula: $C_{25}H_{49}O_{10}P$) (labeled as "Ligand of Interest" by depositor).

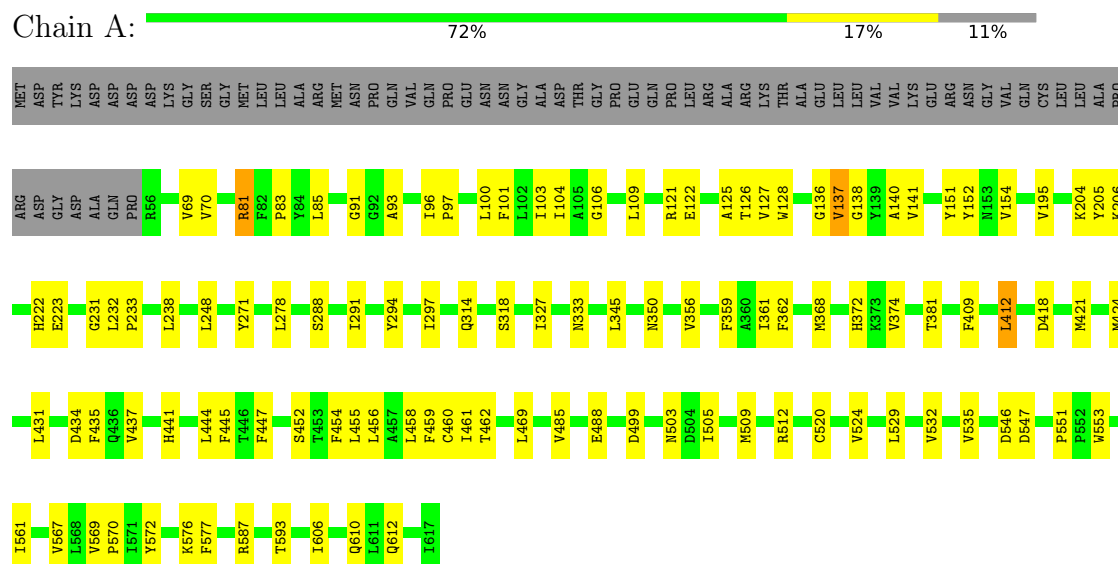


Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	O	P	0
			36	25	10	1	
4	B	1	Total	C	O	P	0
			36	25	10	1	

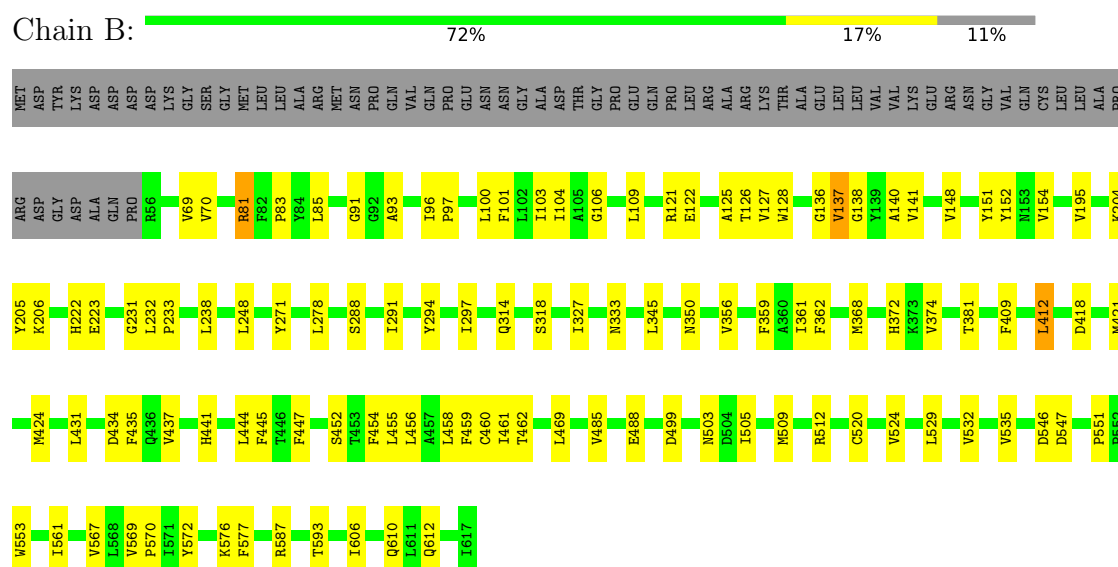
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Sodium-dependent noradrenaline transporter



- Molecule 1: Sodium-dependent noradrenaline transporter



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	200579	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1EFM, A1D5S, CLR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.36	0/4615	0.50	0/6298
1	B	0.36	0/4615	0.50	0/6298
All	All	0.36	0/9230	0.50	0/12596

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4470	0	4423	113	0
1	B	4470	0	4423	114	0
2	A	196	0	322	79	0
2	B	196	0	322	78	0
3	A	33	0	0	0	0
3	B	33	0	0	1	0
4	A	36	0	0	3	0
4	B	36	0	0	3	0
All	All	9470	0	9490	257	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (257) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:LEU:CD1	2:B:704:CLR:H273	1.61	1.30
1:A:456:LEU:CD1	2:A:706:CLR:H273	1.61	1.29
1:B:447:PHE:CD1	2:B:702:CLR:H213	1.74	1.21
1:A:447:PHE:CD1	2:A:704:CLR:H213	1.75	1.20
1:B:456:LEU:HD11	2:B:704:CLR:C27	1.77	1.14
1:A:456:LEU:HD11	2:A:706:CLR:C27	1.77	1.13
1:B:447:PHE:CE1	2:B:702:CLR:H17	1.93	1.04
1:A:456:LEU:HD11	2:A:706:CLR:H273	1.04	1.03
1:B:456:LEU:HD11	2:B:704:CLR:H273	1.04	1.03
1:A:447:PHE:CE1	2:A:704:CLR:H17	1.93	1.03
1:B:561:ILE:HD11	2:B:704:CLR:H181	1.41	1.03
1:A:561:ILE:HD11	2:A:706:CLR:H181	1.41	1.02
1:A:447:PHE:HD1	2:A:704:CLR:H213	1.30	0.90
1:B:447:PHE:HD1	2:B:702:CLR:H213	1.29	0.89
2:A:701:CLR:H17	2:B:708:CLR:H17	1.54	0.88
1:B:447:PHE:CE1	2:B:702:CLR:H213	2.10	0.87
1:B:447:PHE:HE1	2:B:702:CLR:H17	1.40	0.86
1:A:447:PHE:CE1	2:A:704:CLR:H213	2.10	0.86
1:A:447:PHE:HE1	2:A:704:CLR:H17	1.39	0.86
1:B:452:SER:HB3	2:B:701:CLR:H273	1.58	0.86
1:B:447:PHE:CD1	2:B:702:CLR:C21	2.59	0.86
1:A:447:PHE:CD1	2:A:704:CLR:C21	2.59	0.85
1:A:452:SER:HB3	2:A:703:CLR:H273	1.58	0.84
1:B:447:PHE:HD1	2:B:702:CLR:C21	1.91	0.84
1:B:459:PHE:CE2	2:B:705:CLR:H151	2.14	0.83
1:A:233:PRO:HD2	2:A:708:CLR:H72	1.61	0.83
1:B:561:ILE:CD1	2:B:704:CLR:H181	2.07	0.83
1:A:561:ILE:CD1	2:A:706:CLR:H181	2.08	0.82
1:A:459:PHE:CE2	2:A:707:CLR:H151	2.14	0.82
1:A:447:PHE:HD1	2:A:704:CLR:C21	1.91	0.81
1:B:233:PRO:HD2	2:B:706:CLR:H72	1.61	0.81
1:A:231:GLY:O	2:A:707:CLR:H41	1.83	0.79
1:B:231:GLY:O	2:B:705:CLR:H41	1.83	0.78
1:A:456:LEU:HD13	2:A:706:CLR:H273	1.66	0.78
1:B:456:LEU:HD13	2:B:704:CLR:H273	1.66	0.78
1:A:569:VAL:HB	1:A:570:PRO:HD3	1.69	0.75
2:A:701:CLR:H221	2:B:708:CLR:H213	1.70	0.74
1:B:238:LEU:HD22	2:B:706:CLR:H193	1.70	0.74
1:B:569:VAL:HB	1:B:570:PRO:HD3	1.69	0.73
2:A:701:CLR:H213	2:B:708:CLR:H221	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:LYS:HG3	1:B:546:ASP:HB3	1.70	0.73
1:B:154:VAL:HG21	1:B:460:CYS:HB2	1.71	0.72
1:A:238:LEU:HD22	2:A:708:CLR:H193	1.71	0.72
1:A:204:LYS:HG3	1:A:546:ASP:HB3	1.70	0.72
1:A:447:PHE:CZ	2:A:705:CLR:H162	2.25	0.72
1:B:447:PHE:CZ	2:B:703:CLR:H162	2.26	0.71
1:A:154:VAL:HG21	1:A:460:CYS:HB2	1.72	0.70
1:A:447:PHE:CE2	2:A:705:CLR:H162	2.26	0.70
1:A:204:LYS:HD2	1:A:381:THR:HA	1.75	0.69
1:B:447:PHE:CE2	2:B:703:CLR:H162	2.26	0.69
1:B:204:LYS:HD2	1:B:381:THR:HA	1.75	0.68
1:B:238:LEU:HD22	2:B:706:CLR:C19	2.25	0.66
1:A:238:LEU:HD22	2:A:708:CLR:C19	2.26	0.65
1:B:437:VAL:HG11	2:B:701:CLR:H21	1.79	0.65
1:B:81:ARG:HB3	1:B:314:GLN:HE22	1.63	0.64
1:A:81:ARG:HB3	1:A:314:GLN:HE22	1.63	0.64
1:B:444:LEU:HD21	2:B:701:CLR:H72	1.81	0.63
1:A:318:SER:HB2	1:A:350:ASN:HD21	1.65	0.62
1:A:437:VAL:HG11	2:A:703:CLR:H21	1.79	0.62
1:A:232:LEU:HB3	2:A:708:CLR:H6	1.81	0.62
1:B:452:SER:HB3	2:B:701:CLR:C27	2.29	0.62
1:A:444:LEU:HD21	2:A:703:CLR:H72	1.81	0.61
1:B:232:LEU:HB3	2:B:706:CLR:H6	1.81	0.61
1:B:444:LEU:CD2	2:B:701:CLR:H8	2.31	0.61
1:A:444:LEU:CD2	2:A:703:CLR:H8	2.31	0.61
1:A:456:LEU:CD1	2:A:706:CLR:C27	2.53	0.61
1:B:318:SER:HB2	1:B:350:ASN:HD21	1.65	0.60
1:A:452:SER:HB3	2:A:703:CLR:C27	2.29	0.60
1:B:278:LEU:HD11	1:B:356:VAL:HB	1.83	0.60
2:A:701:CLR:H14	2:B:708:CLR:H122	1.85	0.59
1:A:278:LEU:HD11	1:A:356:VAL:HB	1.83	0.58
2:A:701:CLR:H122	2:B:708:CLR:H14	1.85	0.58
1:A:83:PRO:HB3	1:A:361:ILE:HG13	1.86	0.58
2:B:705:CLR:H191	2:B:706:CLR:H151	1.86	0.58
2:A:707:CLR:H191	2:A:708:CLR:H151	1.86	0.58
1:A:137:VAL:HG12	1:A:569:VAL:HG13	1.86	0.58
1:B:137:VAL:HG12	1:B:569:VAL:HG13	1.86	0.58
1:A:447:PHE:CZ	2:A:705:CLR:C16	2.86	0.57
1:A:505:ILE:HG23	1:A:509:MET:HE3	1.86	0.57
1:A:85:LEU:HD12	1:A:314:GLN:HE21	1.68	0.57
1:B:505:ILE:HG23	1:B:509:MET:HE3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:PRO:HB3	1:B:461:ILE:HG13	1.86	0.57
1:B:103:ILE:HG13	1:B:104:ILE:HG23	1.86	0.57
1:B:447:PHE:CZ	2:B:703:CLR:C16	2.87	0.57
1:B:520:CYS:HA	1:B:524:VAL:HB	1.87	0.57
1:A:103:ILE:HG13	1:A:104:ILE:HG23	1.87	0.56
1:A:127:VAL:HG11	1:A:327:ILE:HD13	1.87	0.56
1:B:85:LEU:HD12	1:B:314:GLN:HE21	1.68	0.56
1:A:233:PRO:HB3	1:A:461:ILE:HG13	1.86	0.56
1:B:83:PRO:HB3	1:B:361:ILE:HG13	1.86	0.56
1:B:447:PHE:CD1	2:B:702:CLR:H17	2.40	0.56
1:B:127:VAL:HG11	1:B:327:ILE:HD13	1.87	0.56
1:B:137:VAL:HG12	1:B:569:VAL:HG22	1.88	0.56
1:A:452:SER:HA	2:A:703:CLR:H271	1.88	0.56
1:B:452:SER:HA	2:B:701:CLR:H271	1.88	0.56
1:A:137:VAL:HG12	1:A:569:VAL:HG22	1.88	0.56
1:A:520:CYS:HA	1:A:524:VAL:HB	1.87	0.55
1:B:437:VAL:HG11	2:B:701:CLR:C2	2.35	0.55
1:A:137:VAL:O	1:A:140:ALA:HB3	2.07	0.55
1:A:418:ASP:HA	1:A:421:MET:HE3	1.89	0.55
1:B:456:LEU:HD13	2:B:704:CLR:H231	1.89	0.55
1:A:437:VAL:HG11	2:A:703:CLR:C2	2.36	0.55
1:B:137:VAL:O	1:B:140:ALA:HB3	2.07	0.54
2:A:703:CLR:H12	2:B:708:CLR:H161	1.90	0.54
1:B:418:ASP:HA	1:B:421:MET:HE3	1.89	0.54
1:B:458:LEU:HD13	2:B:706:CLR:H162	1.90	0.54
1:A:456:LEU:HD13	2:A:706:CLR:H231	1.89	0.54
2:A:701:CLR:H161	2:B:701:CLR:H12	1.90	0.54
1:A:447:PHE:HE1	2:A:704:CLR:C17	2.15	0.53
1:B:447:PHE:CE1	2:B:703:CLR:H161	2.44	0.53
1:B:577:PHE:O	1:B:587:ARG:NH2	2.40	0.53
1:A:447:PHE:CE1	2:A:705:CLR:H161	2.43	0.53
1:A:458:LEU:HD13	2:A:708:CLR:H162	1.90	0.53
1:A:206:LYS:NZ	1:A:547:ASP:OD2	2.42	0.53
1:B:456:LEU:HD21	2:B:705:CLR:H25	1.91	0.53
2:A:703:CLR:H261	2:A:707:CLR:H273	1.91	0.52
1:B:121:ARG:NH2	1:B:333:ASN:O	2.42	0.52
1:B:238:LEU:CD2	2:B:706:CLR:H193	2.38	0.52
1:A:238:LEU:CD2	2:A:708:CLR:H193	2.38	0.52
1:A:409:PHE:HA	1:A:412:LEU:CD2	2.40	0.52
1:A:434:ASP:OD1	4:A:709:A1EFM:C33	2.57	0.52
1:B:456:LEU:CD1	2:B:704:CLR:C27	2.53	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:701:CLR:H261	2:B:705:CLR:H273	1.91	0.52
1:A:447:PHE:CZ	2:A:705:CLR:H222	2.44	0.52
2:A:701:CLR:C16	2:B:701:CLR:H12	2.39	0.52
2:A:703:CLR:H71	4:B:707:A1EFM:O10	2.10	0.52
1:B:532:VAL:HA	1:B:535:VAL:HG22	1.92	0.52
1:A:456:LEU:HD21	2:A:707:CLR:H25	1.90	0.52
1:B:409:PHE:HA	1:B:412:LEU:CD2	2.40	0.52
1:B:434:ASP:OD1	4:B:707:A1EFM:C33	2.58	0.52
1:B:447:PHE:CE1	2:B:702:CLR:C21	2.90	0.52
1:B:441:HIS:CE1	2:B:701:CLR:H42	2.44	0.52
1:B:447:PHE:CZ	2:B:703:CLR:H222	2.44	0.52
1:A:441:HIS:CE1	2:A:703:CLR:H42	2.45	0.52
4:A:709:A1EFM:O10	2:B:701:CLR:H71	2.10	0.52
2:A:703:CLR:H12	2:B:708:CLR:C16	2.39	0.52
1:B:233:PRO:HA	1:B:462:THR:HA	1.92	0.51
1:B:447:PHE:HE1	2:B:702:CLR:C17	2.15	0.51
2:B:705:CLR:H183	2:B:706:CLR:H241	1.93	0.51
1:A:577:PHE:O	1:A:587:ARG:NH2	2.40	0.51
2:A:707:CLR:H183	2:A:708:CLR:H241	1.93	0.51
1:A:121:ARG:NH2	1:A:333:ASN:O	2.42	0.51
1:B:128:TRP:HZ2	1:B:488:GLU:HG2	1.76	0.51
1:A:205:TYR:HE2	1:A:372:HIS:HB3	1.76	0.51
1:A:233:PRO:HA	1:A:462:THR:HA	1.92	0.51
1:A:532:VAL:HA	1:A:535:VAL:HG22	1.92	0.51
1:A:567:VAL:C	1:A:570:PRO:HD2	2.36	0.51
1:B:206:LYS:NZ	1:B:547:ASP:OD2	2.42	0.51
1:A:447:PHE:CD1	2:A:704:CLR:H17	2.41	0.51
1:B:567:VAL:C	1:B:570:PRO:HD2	2.36	0.50
1:A:128:TRP:HZ2	1:A:488:GLU:HG2	1.76	0.50
1:A:409:PHE:HA	1:A:412:LEU:HD23	1.94	0.49
1:B:101:PHE:O	1:B:106:GLY:N	2.37	0.49
1:B:593:THR:HG21	1:B:606:ILE:HD12	1.95	0.49
1:B:205:TYR:HE2	1:B:372:HIS:HB3	1.76	0.49
1:A:455:LEU:HD22	2:A:708:CLR:H242	1.95	0.49
1:B:125:ALA:HA	1:B:138:GLY:HA3	1.94	0.49
1:A:125:ALA:HA	1:A:138:GLY:HA3	1.94	0.48
1:A:593:THR:HG21	1:A:606:ILE:HD12	1.95	0.48
1:A:610:GLN:NE2	1:A:612:GLN:OE1	2.46	0.48
2:A:704:CLR:H9	2:A:705:CLR:H14	1.94	0.48
1:B:409:PHE:HA	1:B:412:LEU:HD23	1.94	0.48
1:B:455:LEU:HD22	2:B:706:CLR:H242	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:702:CLR:H9	2:B:703:CLR:H14	1.94	0.48
1:B:610:GLN:NE2	1:B:612:GLN:OE1	2.46	0.47
1:A:447:PHE:CE1	2:A:704:CLR:C21	2.90	0.47
1:B:503:ASN:OD1	1:B:512:ARG:NH2	2.47	0.47
1:A:503:ASN:OD1	1:A:512:ARG:NH2	2.47	0.47
1:A:248:LEU:HD21	1:A:424:MET:HG3	1.97	0.47
1:B:444:LEU:HD23	2:B:701:CLR:H8	1.97	0.47
1:B:368:MET:O	1:B:372:HIS:ND1	2.42	0.46
1:A:70:VAL:HB	1:A:271:TYR:HE2	1.80	0.46
1:B:70:VAL:HB	1:B:271:TYR:HE2	1.80	0.46
1:B:96:ILE:HB	1:B:97:PRO:HD3	1.98	0.46
1:B:431:LEU:HD12	1:B:445:PHE:HZ	1.80	0.46
1:B:69:VAL:HG11	1:B:345:LEU:HD23	1.98	0.46
1:B:454:PHE:O	1:B:458:LEU:HG	2.16	0.46
1:A:437:VAL:CG1	2:A:703:CLR:H22	2.46	0.46
1:A:96:ILE:HB	1:A:97:PRO:HD3	1.98	0.46
1:A:291:ILE:HG23	1:A:359:PHE:CE1	2.51	0.46
2:A:706:CLR:H6	2:B:705:CLR:H12	1.98	0.46
1:B:459:PHE:CE2	2:B:705:CLR:C15	2.95	0.46
1:B:291:ILE:HG23	1:B:359:PHE:CE1	2.51	0.45
1:B:437:VAL:CG1	2:B:701:CLR:H22	2.46	0.45
1:A:431:LEU:HD12	1:A:445:PHE:HZ	1.80	0.45
1:A:444:LEU:HD23	2:A:703:CLR:H8	1.97	0.45
1:A:151:TYR:HB2	1:A:469:LEU:HG	1.99	0.45
1:B:248:LEU:HD21	1:B:424:MET:HG3	1.97	0.45
1:A:69:VAL:HG11	1:A:345:LEU:HD23	1.98	0.45
1:A:454:PHE:O	1:A:458:LEU:HG	2.16	0.45
1:A:109:LEU:HD11	1:A:529:LEU:HD11	1.99	0.44
2:A:707:CLR:H12	2:B:704:CLR:H6	1.98	0.44
1:A:101:PHE:O	1:A:106:GLY:N	2.37	0.44
1:A:222:HIS:CE1	1:A:223:GLU:HG3	2.53	0.44
2:A:701:CLR:H222	2:A:701:CLR:H162	1.78	0.44
1:B:151:TYR:HB2	1:B:469:LEU:HG	1.99	0.44
1:B:551:PRO:HB2	1:B:553:TRP:CD1	2.53	0.44
1:B:572:TYR:HE1	4:B:707:A1EFM:C25	2.31	0.44
1:A:100:LEU:O	1:A:104:ILE:HG12	2.18	0.43
1:A:444:LEU:HD23	2:A:703:CLR:H191	2.00	0.43
1:A:551:PRO:HB2	1:A:553:TRP:CD1	2.53	0.43
1:B:222:HIS:CE1	1:B:223:GLU:HG3	2.53	0.43
1:B:109:LEU:HD11	1:B:529:LEU:HD11	1.99	0.43
1:B:100:LEU:O	1:B:104:ILE:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:SER:HA	1:B:291:ILE:HD12	2.01	0.43
1:A:572:TYR:HE1	4:A:709:A1EFM:C25	2.31	0.43
2:B:704:CLR:H261	2:B:705:CLR:H261	2.00	0.43
2:A:701:CLR:H71	2:B:701:CLR:H122	2.01	0.43
1:A:138:GLY:O	1:A:141:VAL:HG22	2.19	0.43
1:A:447:PHE:HE1	2:A:704:CLR:H221	1.84	0.43
1:B:447:PHE:HE1	2:B:702:CLR:H221	1.84	0.43
1:A:444:LEU:HD21	2:A:703:CLR:C7	2.49	0.42
1:A:455:LEU:CD1	2:A:707:CLR:H241	2.49	0.42
1:A:459:PHE:CE2	2:A:707:CLR:C15	2.95	0.42
2:A:706:CLR:H261	2:A:707:CLR:H261	2.00	0.42
1:B:444:LEU:HD23	2:B:701:CLR:H191	2.00	0.42
1:A:93:ALA:HA	1:A:297:ILE:HG23	2.02	0.42
1:B:455:LEU:CD1	2:B:705:CLR:H241	2.49	0.42
1:B:93:ALA:HA	1:B:297:ILE:HG23	2.02	0.42
1:B:138:GLY:O	1:B:141:VAL:HG22	2.19	0.42
2:A:703:CLR:H122	2:B:708:CLR:H71	2.01	0.42
1:B:459:PHE:CZ	2:B:705:CLR:H151	2.55	0.42
1:A:288:SER:HA	1:A:291:ILE:HD12	2.01	0.41
1:B:91:GLY:HA3	1:B:362:PHE:CZ	2.55	0.41
1:A:91:GLY:HA3	1:A:362:PHE:CZ	2.55	0.41
1:A:368:MET:O	1:A:372:HIS:ND1	2.42	0.41
1:B:294:TYR:HB2	1:B:362:PHE:CG	2.55	0.41
2:A:701:CLR:H122	2:B:708:CLR:H122	2.02	0.41
1:B:444:LEU:HD21	2:B:701:CLR:C7	2.49	0.41
1:A:459:PHE:CZ	2:A:707:CLR:H151	2.55	0.41
1:B:437:VAL:HG12	2:B:701:CLR:H22	2.02	0.41
1:B:447:PHE:CE1	2:B:703:CLR:C16	3.04	0.41
1:A:485:VAL:HG23	1:A:529:LEU:HD13	2.03	0.41
1:B:485:VAL:HG23	1:B:529:LEU:HD13	2.03	0.41
1:A:294:TYR:HB2	1:A:362:PHE:CG	2.55	0.41
1:A:447:PHE:CE1	2:A:705:CLR:C16	3.03	0.41
1:A:455:LEU:HB3	2:A:707:CLR:H222	2.03	0.41
2:A:703:CLR:H9	2:B:708:CLR:H151	2.03	0.41
1:A:455:LEU:CD2	2:A:708:CLR:H242	2.51	0.41
2:A:704:CLR:H122	2:A:705:CLR:H151	2.03	0.41
1:A:136:GLY:HA3	1:A:572:TYR:CB	2.51	0.41
1:A:553:TRP:CE3	2:B:705:CLR:H21	2.56	0.41
2:A:707:CLR:H21	1:B:553:TRP:CE3	2.56	0.41
1:B:435:PHE:CD2	2:B:708:CLR:H181	2.56	0.41
1:B:455:LEU:CD2	2:B:706:CLR:H242	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:499:ASP:OD1	1:B:499:ASP:N	2.54	0.41
2:B:702:CLR:H122	2:B:703:CLR:H151	2.03	0.41
1:A:233:PRO:HD2	2:A:708:CLR:C7	2.42	0.40
1:A:122:GLU:HB3	1:A:126:THR:OG1	2.21	0.40
1:A:437:VAL:HG12	2:A:703:CLR:H22	2.03	0.40
1:A:435:PHE:CD2	2:A:701:CLR:H181	2.56	0.40
1:B:437:VAL:CG1	2:B:701:CLR:C2	2.99	0.40
1:B:136:GLY:HA3	1:B:572:TYR:CB	2.51	0.40
1:A:499:ASP:OD1	1:A:499:ASP:N	2.54	0.40
1:B:122:GLU:HB3	1:B:126:THR:OG1	2.21	0.40
1:B:148:VAL:HG11	3:B:709:A1D5S:C20	2.52	0.40
1:B:452:SER:CB	2:B:701:CLR:C27	2.99	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	560/629 (89%)	551 (98%)	9 (2%)	0	100	100
1	B	560/629 (89%)	551 (98%)	9 (2%)	0	100	100
All	All	1120/1258 (89%)	1102 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	467/529 (88%)	460 (98%)	7 (2%)	60	80
1	B	467/529 (88%)	460 (98%)	7 (2%)	60	80
All	All	934/1058 (88%)	920 (98%)	14 (2%)	60	80

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	ARG
1	A	137	VAL
1	A	152	TYR
1	A	195	VAL
1	A	374	VAL
1	A	412	LEU
1	A	576	LYS
1	B	81	ARG
1	B	137	VAL
1	B	152	TYR
1	B	195	VAL
1	B	374	VAL
1	B	412	LEU
1	B	576	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	ASN
1	A	170	ASN
1	A	184	ASN
1	A	234	GLN
1	A	280	HIS
1	A	314	GLN
1	A	337	ASN
1	A	350	ASN
1	A	507	GLN
1	A	539	ASN
1	A	610	GLN
1	A	612	GLN
1	B	89	ASN
1	B	170	ASN

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Mol	Chain	Res	Type
1	B	184	ASN
1	B	222	HIS
1	B	314	GLN
1	B	337	ASN
1	B	350	ASN
1	B	539	ASN
1	B	610	GLN
1	B	612	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

18 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	CLR	A	704	-	31,31,31	0.27	0	48,48,48	0.40	0
2	CLR	A	708	-	31,31,31	0.28	0	48,48,48	0.38	0
3	A1D5S	B	709	-	36,36,36	0.47	0	47,47,47	0.39	0
2	CLR	A	703	-	31,31,31	0.29	0	48,48,48	0.43	0
2	CLR	B	702	-	31,31,31	0.27	0	48,48,48	0.40	0
2	CLR	A	707	-	31,31,31	0.26	0	48,48,48	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CLR	A	701	-	31,31,31	0.34	0	48,48,48	0.52	0
2	CLR	B	703	-	31,31,31	0.27	0	48,48,48	0.40	0
2	CLR	B	706	-	31,31,31	0.28	0	48,48,48	0.37	0
2	CLR	B	708	-	31,31,31	0.34	0	48,48,48	0.52	0
3	A1D5S	A	702	-	36,36,36	0.47	0	47,47,47	0.39	0
4	A1EFM	B	707	-	35,35,35	1.03	4 (11%)	38,41,41	1.05	2 (5%)
2	CLR	B	704	-	31,31,31	0.28	0	48,48,48	0.38	0
2	CLR	A	706	-	31,31,31	0.28	0	48,48,48	0.39	0
2	CLR	B	705	-	31,31,31	0.26	0	48,48,48	0.39	0
2	CLR	A	705	-	31,31,31	0.27	0	48,48,48	0.40	0
2	CLR	B	701	-	31,31,31	0.28	0	48,48,48	0.43	0
4	A1EFM	A	709	-	35,35,35	1.02	4 (11%)	38,41,41	1.05	2 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CLR	A	704	-	-	0/10/68/68	0/4/4/4
2	CLR	A	708	-	-	6/10/68/68	0/4/4/4
3	A1D5S	B	709	-	-	11/20/30/30	0/4/4/4
2	CLR	A	703	-	-	4/10/68/68	0/4/4/4
2	CLR	B	702	-	-	0/10/68/68	0/4/4/4
2	CLR	A	707	-	-	4/10/68/68	0/4/4/4
2	CLR	A	701	-	-	0/10/68/68	0/4/4/4
2	CLR	B	703	-	-	4/10/68/68	0/4/4/4
2	CLR	B	706	-	-	6/10/68/68	0/4/4/4
2	CLR	B	708	-	-	0/10/68/68	0/4/4/4
3	A1D5S	A	702	-	-	11/20/30/30	0/4/4/4
4	A1EFM	B	707	-	-	18/40/40/40	-
2	CLR	B	704	-	-	1/10/68/68	0/4/4/4
2	CLR	A	706	-	-	1/10/68/68	0/4/4/4
2	CLR	B	705	-	-	4/10/68/68	0/4/4/4
2	CLR	A	705	-	-	4/10/68/68	0/4/4/4
2	CLR	B	701	-	-	4/10/68/68	0/4/4/4
4	A1EFM	A	709	-	-	18/40/40/40	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	709	A1EFM	O13-C12	-2.55	1.40	1.46
4	B	707	A1EFM	O13-C12	-2.55	1.40	1.46
4	A	709	A1EFM	O10-C09	2.32	1.40	1.33
4	B	707	A1EFM	O10-C09	2.32	1.40	1.33
4	B	707	A1EFM	O10-C11	-2.21	1.40	1.45
4	A	709	A1EFM	O10-C11	-2.18	1.40	1.45
4	B	707	A1EFM	O13-C14	2.17	1.40	1.34
4	A	709	A1EFM	O13-C14	2.15	1.40	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	709	A1EFM	O13-C14-C15	4.24	120.64	111.50
4	B	707	A1EFM	O13-C14-C15	4.23	120.61	111.50
4	A	709	A1EFM	O10-C09-C08	2.51	119.80	111.91
4	B	707	A1EFM	O10-C09-C08	2.51	119.80	111.91

There are no chirality outliers.

All (96) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	702	A1D5S	C09-C10-N11-C16
3	A	702	A1D5S	C26-C07-O08-C09
3	A	702	A1D5S	C04-C07-O08-C09
3	B	709	A1D5S	C09-C10-N11-C16
3	B	709	A1D5S	C26-C07-O08-C09
3	B	709	A1D5S	C04-C07-O08-C09
4	A	709	A1EFM	C25-O26-P27-O28
4	A	709	A1EFM	C30-O29-P27-O35
4	B	707	A1EFM	C25-O26-P27-O28
4	B	707	A1EFM	C30-O29-P27-O35
3	A	702	A1D5S	C18-C17-N14-C15
3	B	709	A1D5S	C18-C17-N14-C15
4	A	709	A1EFM	C08-C09-O10-C11
4	B	707	A1EFM	C08-C09-O10-C11
4	A	709	A1EFM	O36-C09-O10-C11
4	B	707	A1EFM	O36-C09-O10-C11
3	A	702	A1D5S	N14-C17-C18-C19
3	B	709	A1D5S	N14-C17-C18-C19
2	A	708	CLR	C17-C20-C22-C23
2	B	706	CLR	C17-C20-C22-C23
3	A	702	A1D5S	C18-C17-N14-C13

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Mol	Chain	Res	Type	Atoms
3	B	709	A1D5S	C18-C17-N14-C13
4	A	709	A1EFM	C25-O26-P27-O29
4	B	707	A1EFM	C25-O26-P27-O29
2	A	705	CLR	C13-C17-C20-C22
2	A	708	CLR	C13-C17-C20-C22
2	B	706	CLR	C13-C17-C20-C22
2	B	703	CLR	C13-C17-C20-C22
4	A	709	A1EFM	C05-C06-C07-C08
4	B	707	A1EFM	C05-C06-C07-C08
4	A	709	A1EFM	C30-C31-C33-O34
4	B	707	A1EFM	C30-C31-C33-O34
4	A	709	A1EFM	O24-C14-O13-C12
4	B	707	A1EFM	O24-C14-O13-C12
4	A	709	A1EFM	C15-C14-O13-C12
4	B	707	A1EFM	C15-C14-O13-C12
2	A	707	CLR	C13-C17-C20-C22
2	B	705	CLR	C13-C17-C20-C22
2	A	705	CLR	C16-C17-C20-C21
2	B	703	CLR	C16-C17-C20-C21
2	A	705	CLR	C13-C17-C20-C21
2	B	703	CLR	C13-C17-C20-C21
3	A	702	A1D5S	C17-C18-C19-C20
3	B	709	A1D5S	C17-C18-C19-C20
3	B	709	A1D5S	O08-C09-C10-N11
3	A	702	A1D5S	O08-C09-C10-N11
2	A	708	CLR	C21-C20-C22-C23
2	B	706	CLR	C21-C20-C22-C23
2	A	708	CLR	C13-C17-C20-C21
2	B	706	CLR	C13-C17-C20-C21
3	A	702	A1D5S	C09-C10-N11-C12
3	B	709	A1D5S	C09-C10-N11-C12
2	A	708	CLR	C16-C17-C20-C21
2	B	706	CLR	C16-C17-C20-C21
2	A	708	CLR	C16-C17-C20-C22
2	B	706	CLR	C16-C17-C20-C22
2	A	705	CLR	C16-C17-C20-C22
2	B	703	CLR	C16-C17-C20-C22
2	A	707	CLR	C13-C17-C20-C21
2	B	705	CLR	C13-C17-C20-C21
2	A	707	CLR	C16-C17-C20-C22
2	B	705	CLR	C16-C17-C20-C22
2	A	707	CLR	C16-C17-C20-C21

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Mol	Chain	Res	Type	Atoms
2	B	705	CLR	C16-C17-C20-C21
4	A	709	A1EFM	C18-C19-C20-C21
4	B	707	A1EFM	C18-C19-C20-C21
4	A	709	A1EFM	C03-C04-C05-C06
4	B	707	A1EFM	C03-C04-C05-C06
4	A	709	A1EFM	C25-O26-P27-O35
4	B	707	A1EFM	C25-O26-P27-O35
2	A	703	CLR	C16-C17-C20-C22
2	B	701	CLR	C16-C17-C20-C22
2	A	703	CLR	C13-C17-C20-C22
2	B	701	CLR	C13-C17-C20-C22
2	A	703	CLR	C13-C17-C20-C21
2	B	701	CLR	C13-C17-C20-C21
2	B	704	CLR	C17-C20-C22-C23
2	A	706	CLR	C17-C20-C22-C23
4	A	709	A1EFM	O32-C31-C33-O34
4	B	707	A1EFM	O32-C31-C33-O34
4	B	707	A1EFM	C16-C17-C18-C19
4	A	709	A1EFM	C16-C17-C18-C19
2	A	703	CLR	C16-C17-C20-C21
2	B	701	CLR	C16-C17-C20-C21
4	A	709	A1EFM	O29-C30-C31-C33
4	B	707	A1EFM	O29-C30-C31-C33
3	A	702	A1D5S	C05-C04-C07-C26
3	B	709	A1D5S	C05-C04-C07-C26
4	A	709	A1EFM	C30-O29-P27-O26
4	B	707	A1EFM	C30-O29-P27-O26
4	A	709	A1EFM	C07-C08-C09-O10
4	B	707	A1EFM	C07-C08-C09-O10
3	A	702	A1D5S	C03-C04-C07-C26
3	B	709	A1D5S	C03-C04-C07-C26
4	A	709	A1EFM	C14-C15-C16-C17
4	B	707	A1EFM	C14-C15-C16-C17

There are no ring outliers.

17 monomers are involved in 147 short contacts:

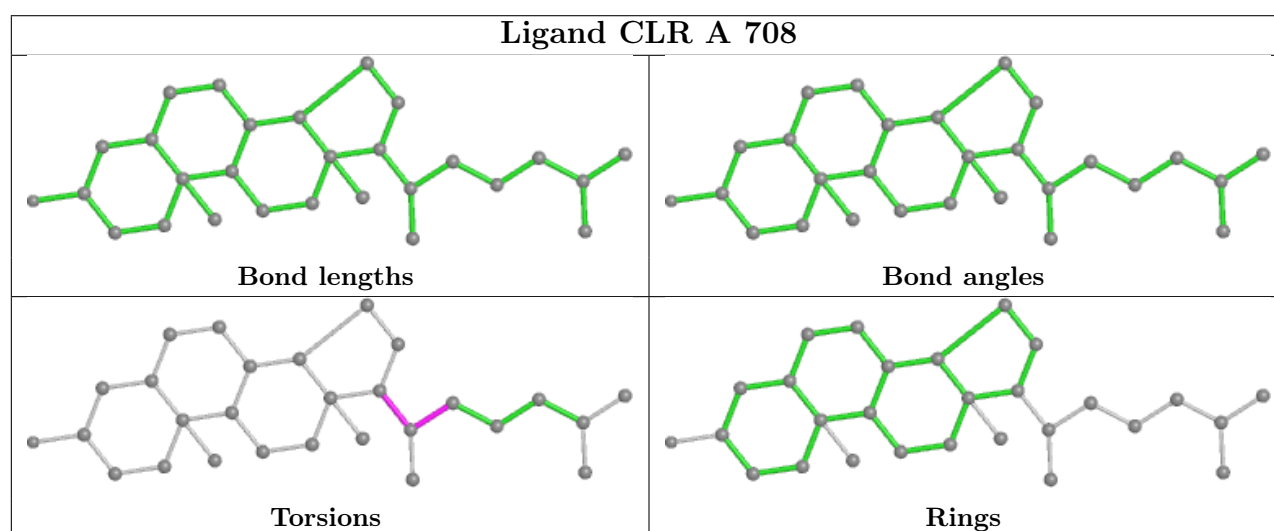
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	704	CLR	13	0
2	A	708	CLR	11	0
3	B	709	A1D5S	1	0
2	A	703	CLR	19	0

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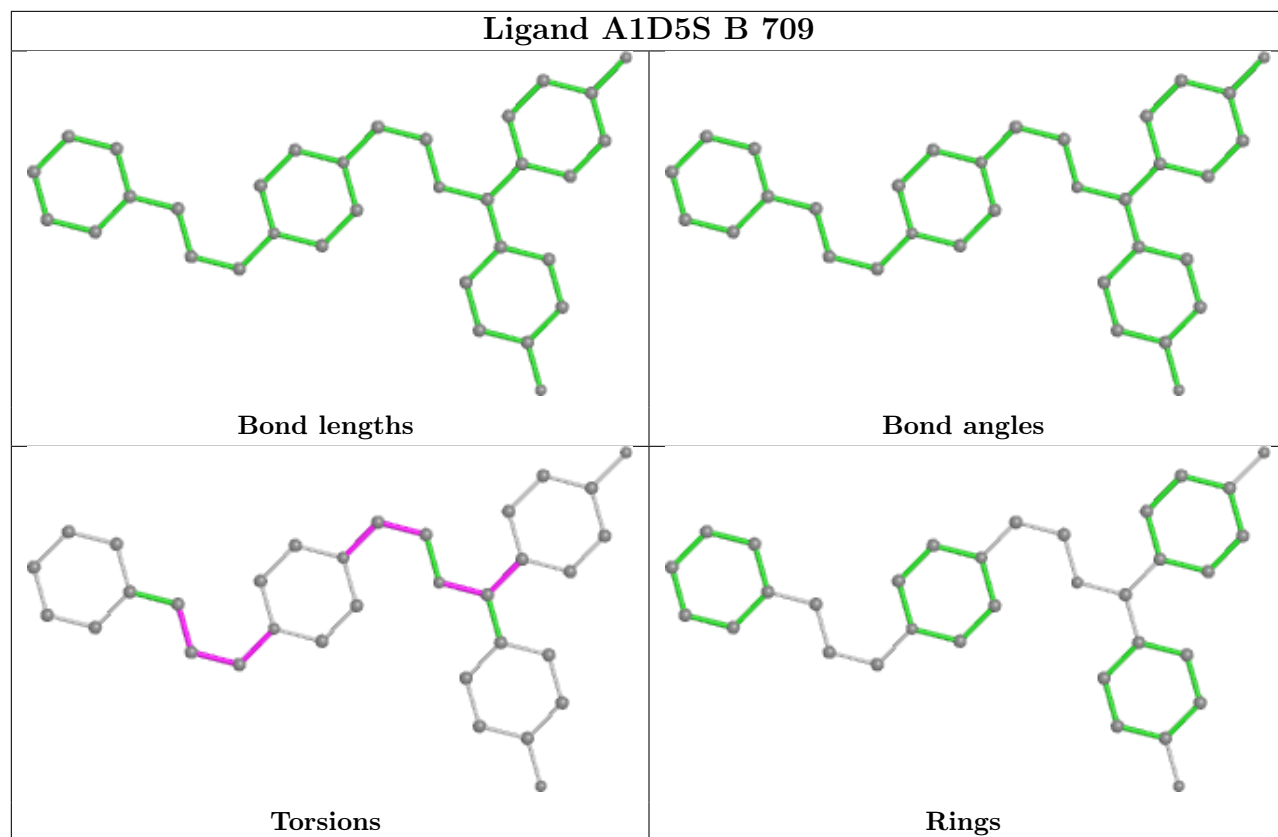
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	702	CLR	13	0
2	A	707	CLR	13	0
2	A	701	CLR	11	0
2	B	703	CLR	8	0
2	B	706	CLR	10	0
2	B	708	CLR	11	0
4	B	707	A1EFM	3	0
2	B	704	CLR	10	0
2	A	706	CLR	10	0
2	B	705	CLR	12	0
2	A	705	CLR	8	0
2	B	701	CLR	20	0
4	A	709	A1EFM	3	0

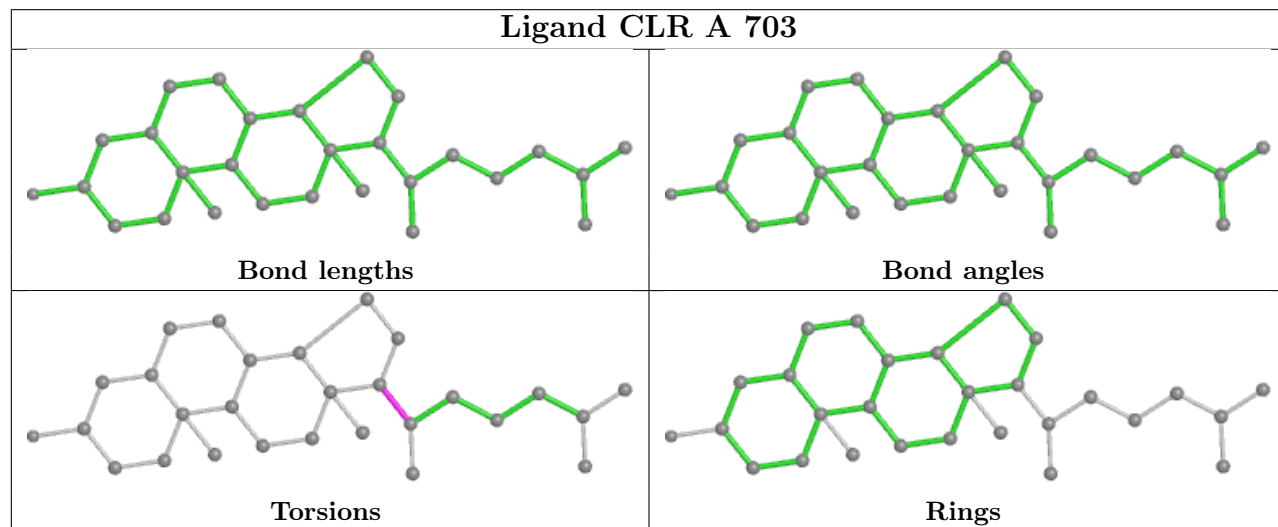
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

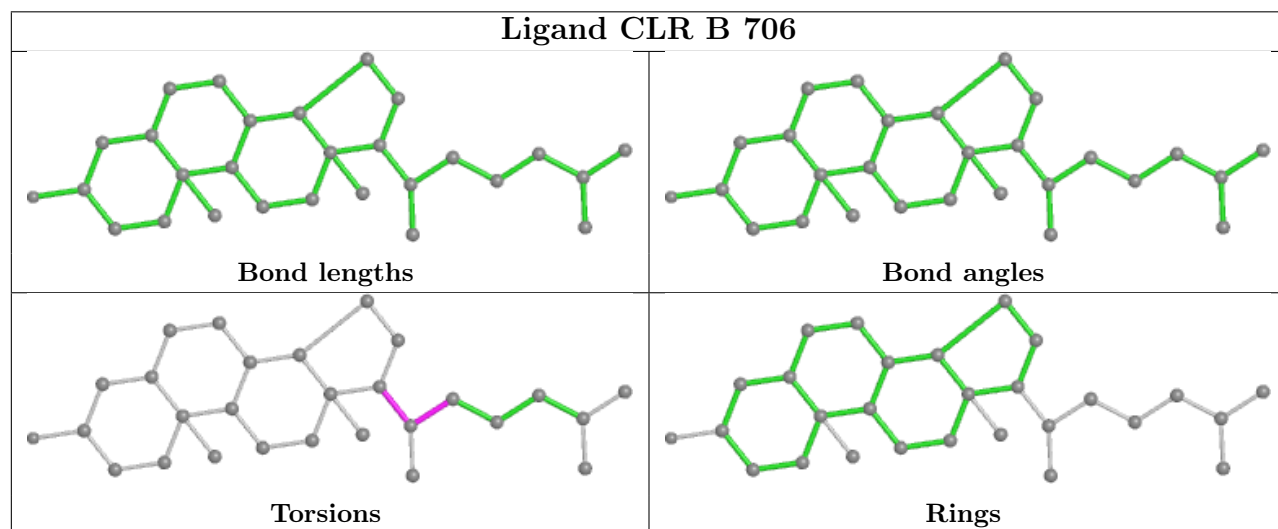
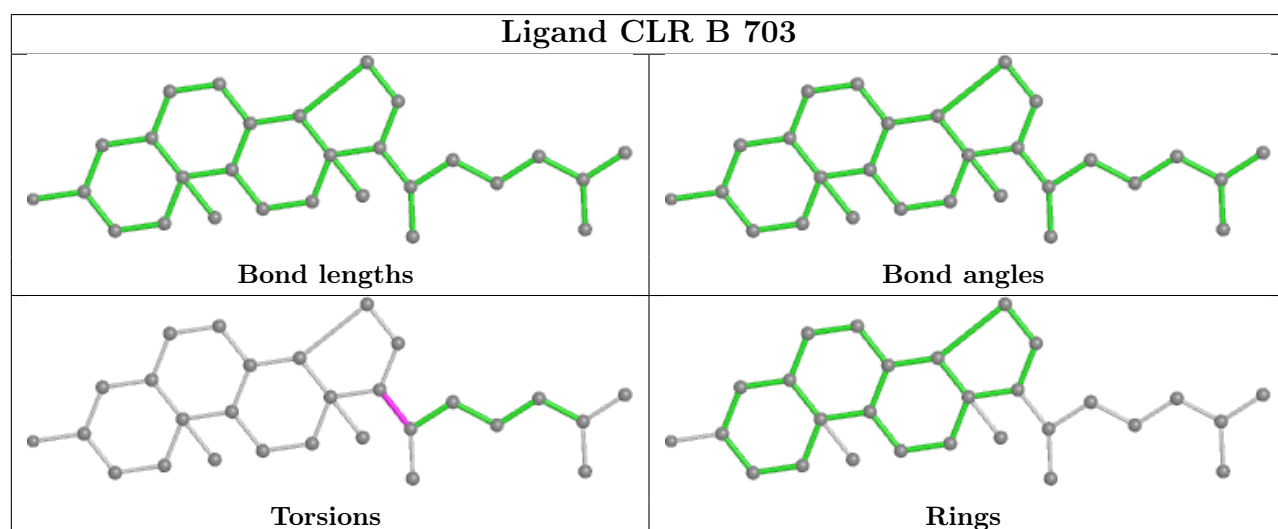
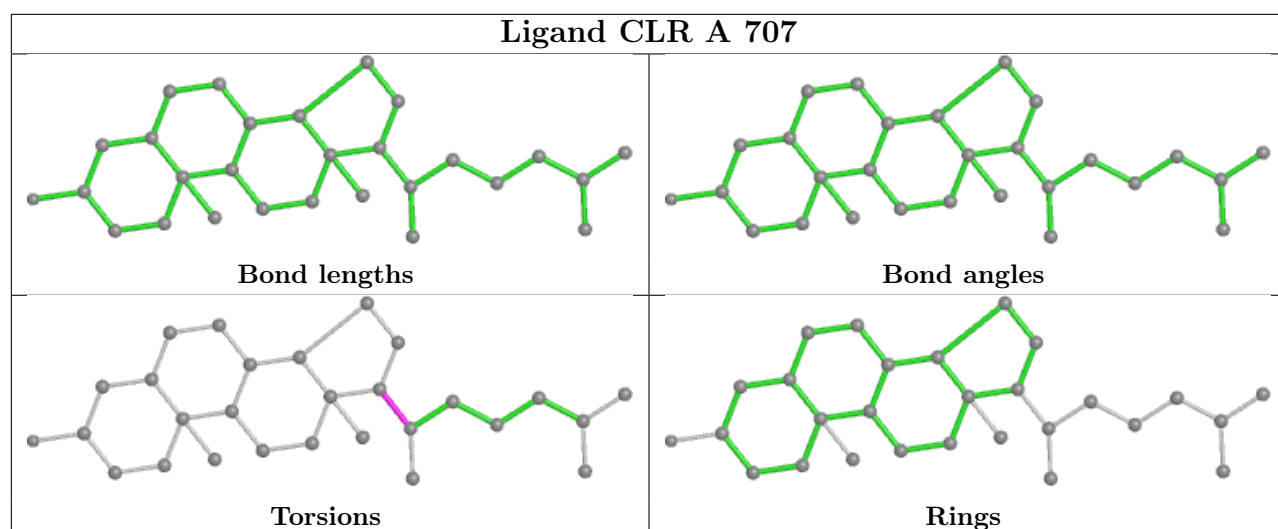


Ligand A1D5S B 709

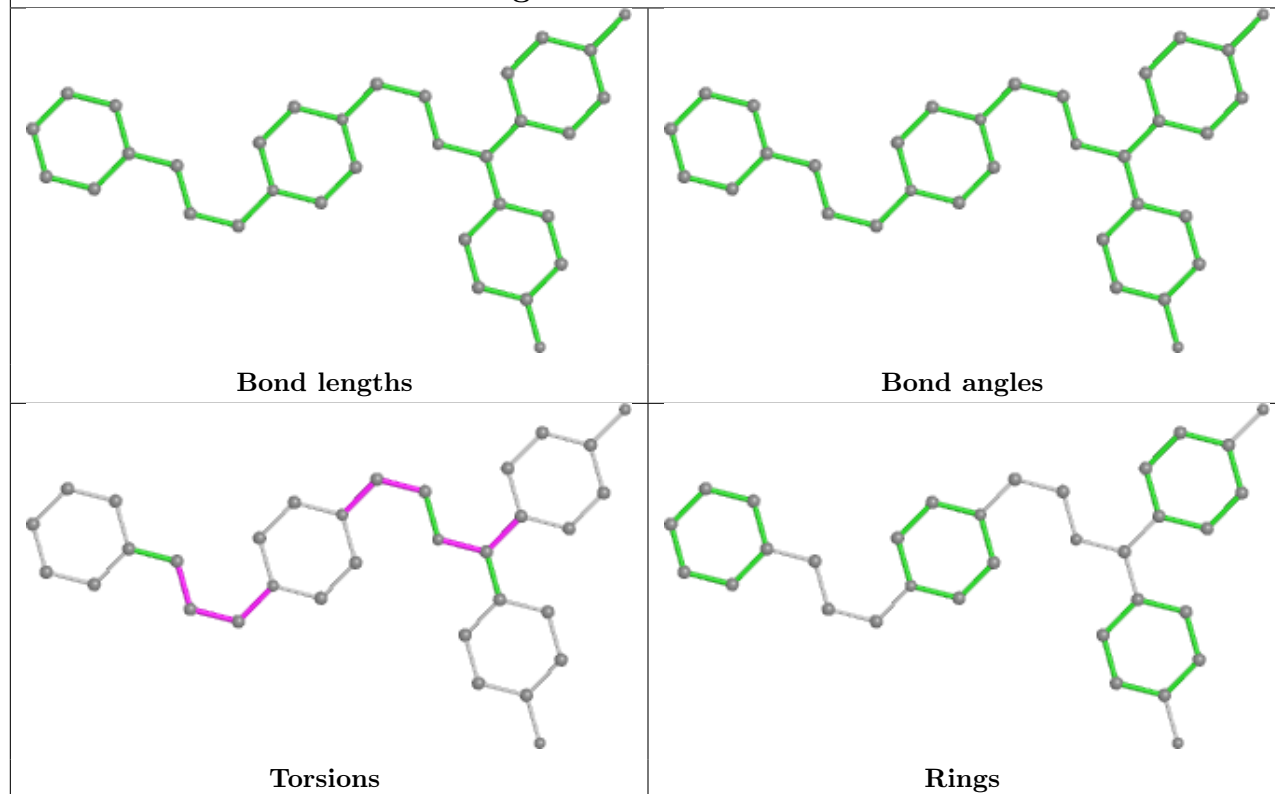


Ligand CLR A 703

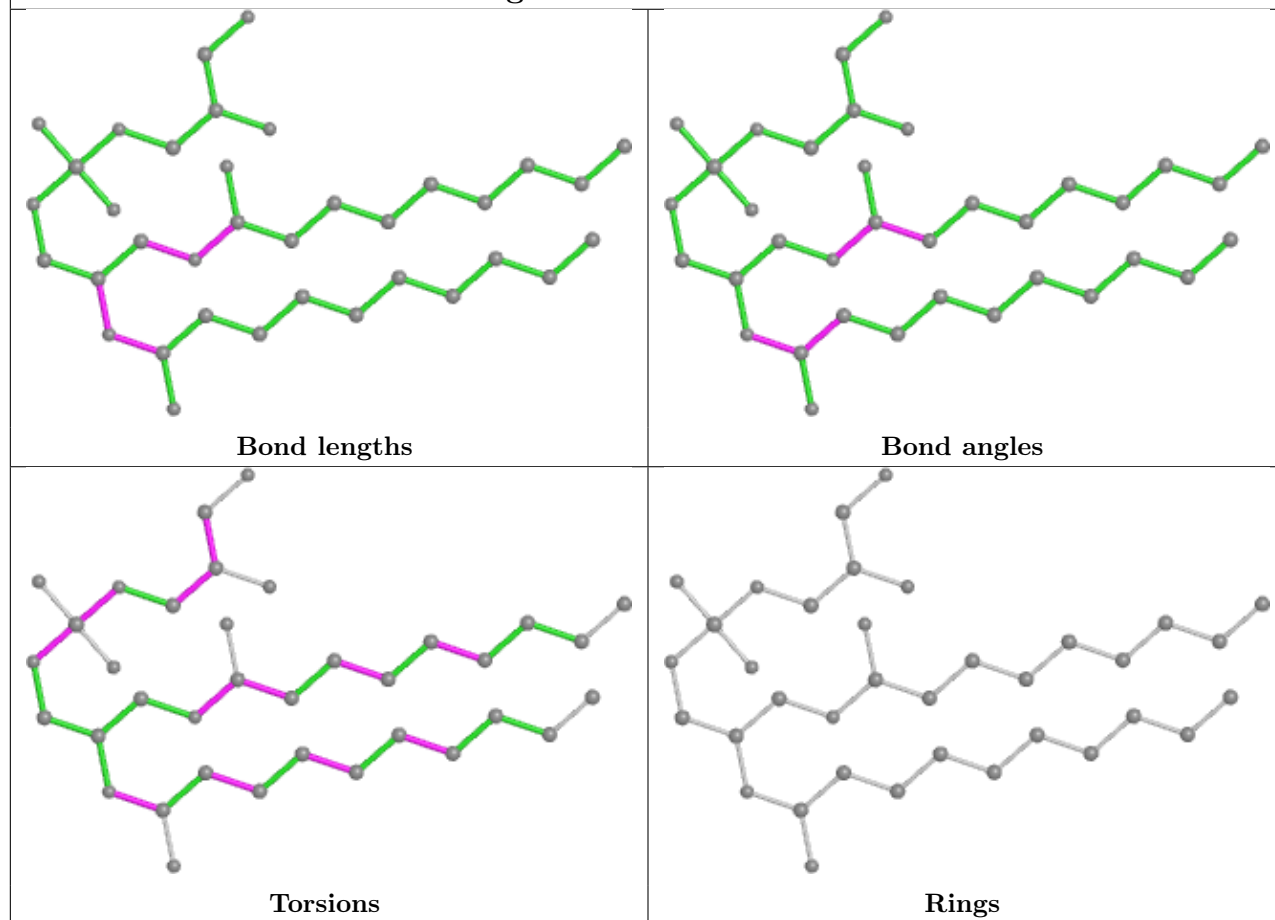




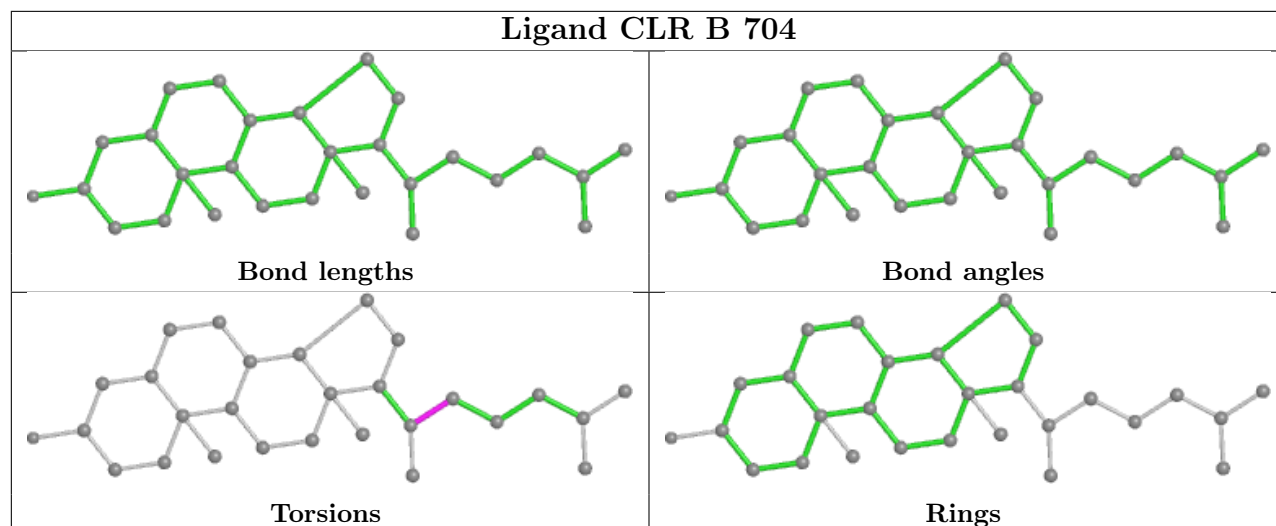
Ligand A1D5S A 702



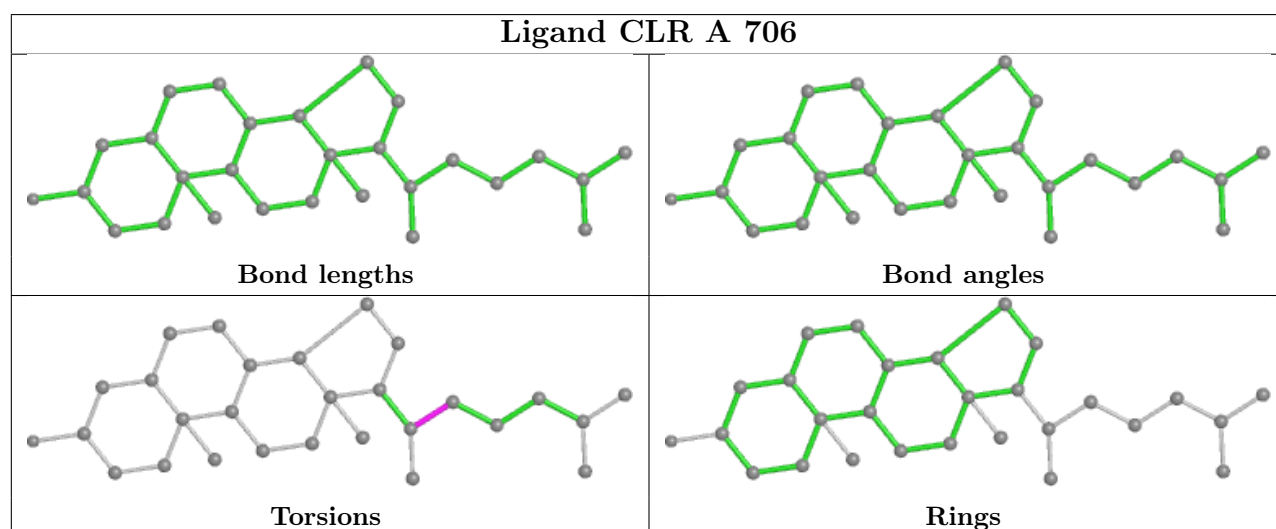
Ligand A1EFM B 707



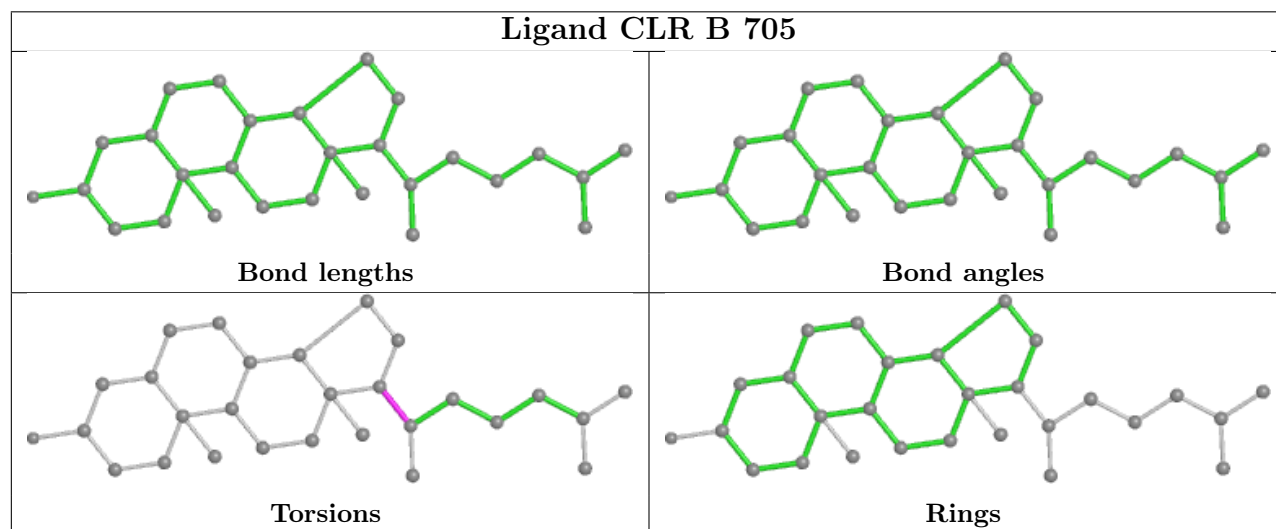
Ligand CLR B 704

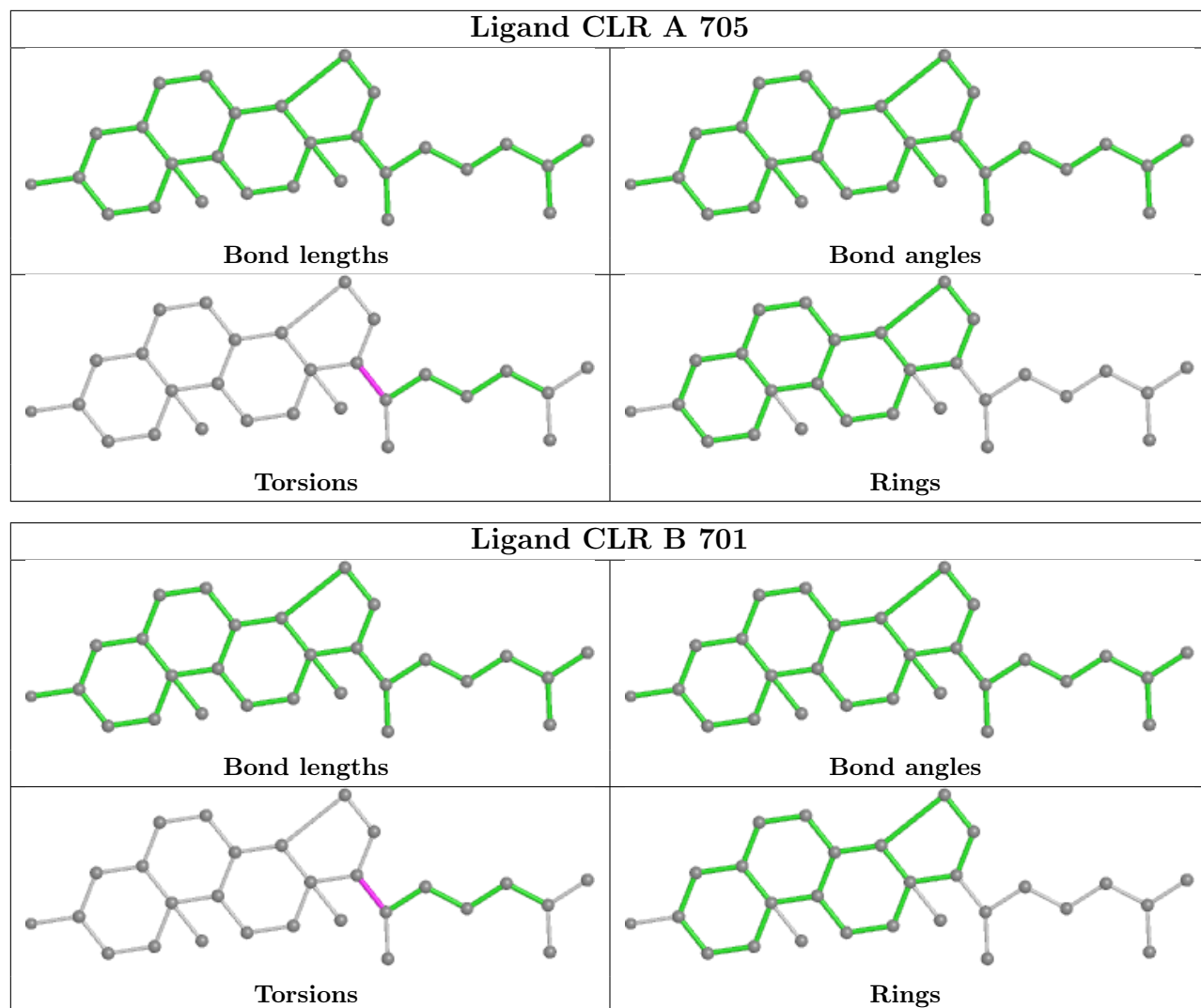


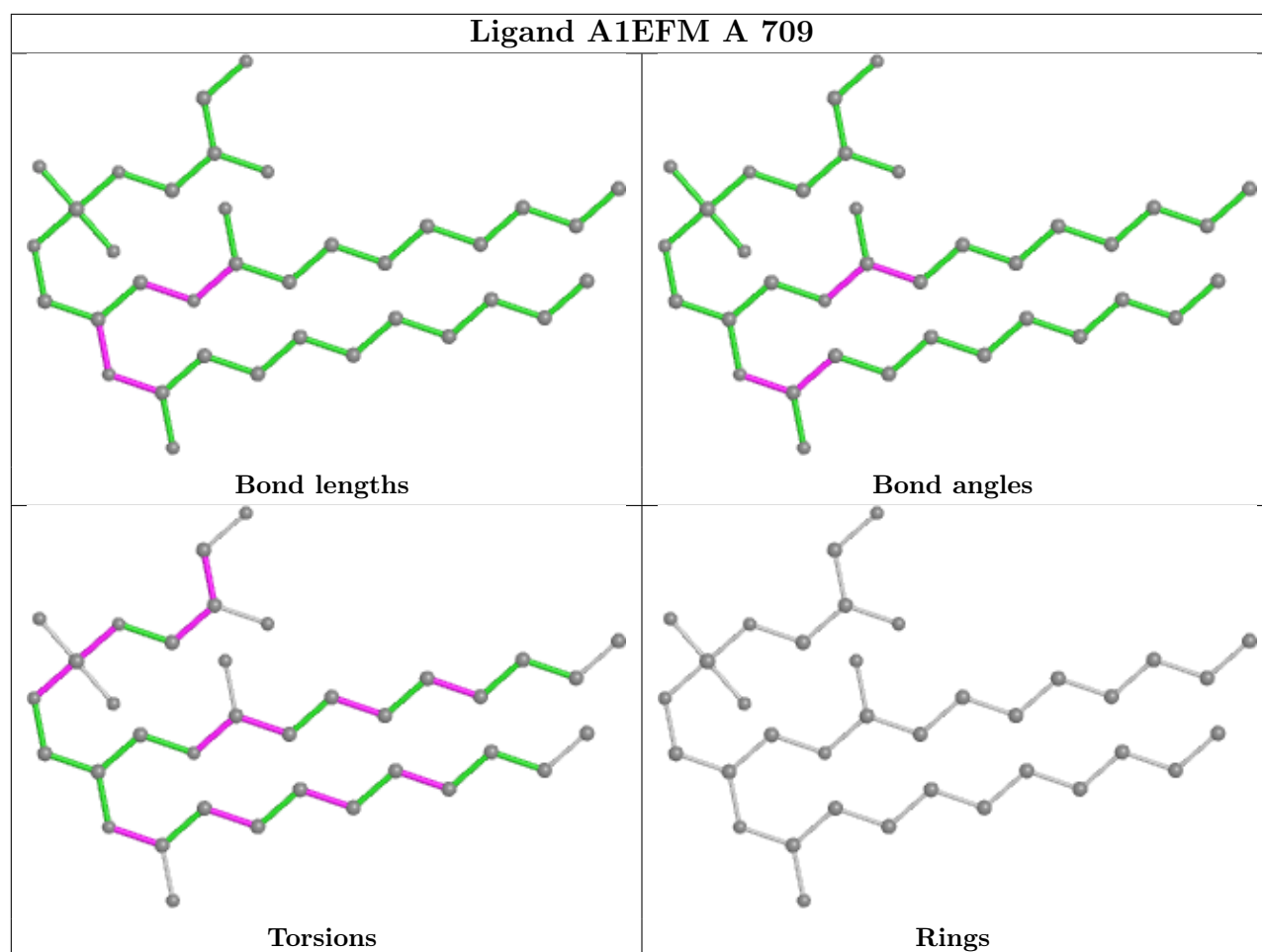
Ligand CLR A 706



Ligand CLR B 705







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.